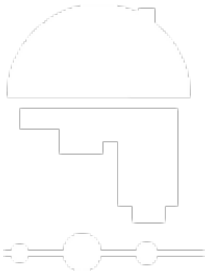

Contribution ID: **9** Type: **Lecture**

Modeling vibrational and electronic spectroscopies with atomic-scale machine learning

Tuesday 16 April 2024 14:15 (1h 30m)

Machine-learning models have greatly extended the scope of application of atomistic simulations, that can evaluate, with predictive accuracy, the stability and properties of materials and molecules. In this lecture, I will briefly overview traditional modeling techniques that can be used to estimate vibrational (IR, Raman, ...) and electronic spectroscopies (optical excitations in particular). I will then discuss how these methods can be combined with data-driven approaches, based on machine-learned approximations of the interatomic potentials and of atomic-scale dielectric and electronic response properties.

Presenter: CERIOTTI, Michele (EPFL Lausanne)